
Bound States of Spherically Symmetric Potentials*

Heat Capacity Calculations

Chandan Kumar

We solve the time-independent Schrödinger equation for spherically symmetric potentials. First, we consider simple cases of a particle on a ring and a particle on a sphere to illustrate the degeneracy arising due to symmetry. We then consider three different spherically symmetric potentials: (i) spherical well potential, (ii) isotropic three-dimensional harmonic oscillator, and (iii) spherically confined isotropic three-dimensional harmonic oscillator. Our discussion mainly focuses on the energy levels of the bound states and the associated degeneracies. Finally, we calculate the heat capacity of endohedral fullerenes using two simple models—particle in a spherical box and confined harmonic oscillator.

1. Introduction

One of the major applications of quantum mechanics is in studying the electronic structure of molecules. The first step involves solving the Schrödinger equation for the electronic molecular Hamiltonian. For many-particle systems, the Schrödinger equation becomes quite complicated, and in many cases, analytical solutions cannot be obtained. In such circumstances, one resorts to numerical methods to solve the Schrödinger equation. Alternatively, a molecular system can be studied by setting up simple quantum models that retain important features.

In recent years, researchers have shown an increased interest in quantum modelling of molecular systems. In this article, we are interested in the quantum modelling of molecular systems



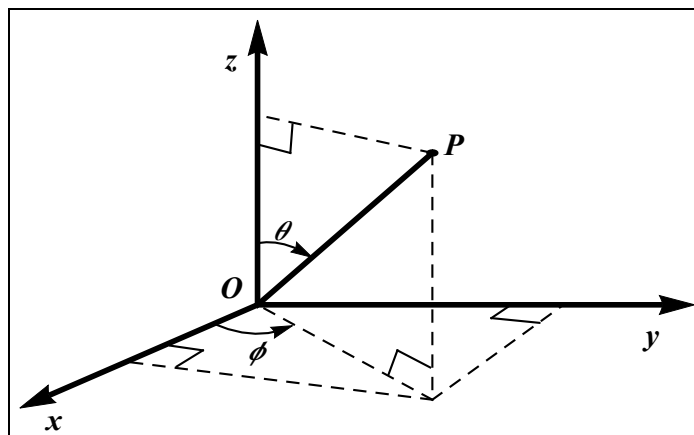
Chandan Kumar is currently pursuing his PhD at IISER Mohali under the guidance of Prof. Arvind. His research interests are quantum optics, continuous variable quantum information theory, and mathematical physics.

Keywords

Schrödinger equation, degeneracy, quantum models.

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Figure 1. Relation between Cartesian coordinates $P(x, y, z)$ and its spherical coordinates $P(r, \theta, \phi)$:
 $x = r \sin \theta \cos \phi$,
 $y = r \sin \theta \sin \phi$,
 $z = r \cos \theta$.



with spherical symmetry. For example, fullerene, a spheroidal molecule, can be modelled as a sphere for studying its properties. We solve the Schrödinger equation for different potentials with spherical symmetry. We obtain the energy levels of the bound states and their degeneracies, which is required to calculate absorption, electrical, and thermodynamic properties.

The material in this paper is organized as follows. Section 2 treats the case of a particle on a ring and a particle on a sphere. Section 3 discusses spherical well potential, isotropic three-dimensional harmonic oscillator, and spherically confined harmonic oscillator. Section 4 presents the quantum modelling of endohedral fullerene and heat capacity calculations. Finally, Section 5 provides some concluding remarks.

2. Schrödinger Equation in Spherical Coordinates

In three dimensions, the time-independent Schrödinger equation in the Cartesian coordinates is written as [1, 2, 3]:

$$-\frac{\hbar^2}{2m_0} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi(x, y, z) + V(x, y, z) \Psi(x, y, z) = E \Psi(x, y, z), \quad (1)$$

where m_0 is the mass of the particle, V is the potential, $\Psi(x, y, z)$ is the time-independent wave function and $\hbar = h/2\pi$ is the reduced Planck's constant. Equation (1) takes the following form in spherical coordinate system (see *Figure 1*):

$$-\frac{\hbar^2}{2m_0} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Psi(r, \theta, \phi) + V(r, \theta, \phi) \Psi(r, \theta, \phi) = E \Psi(r, \theta, \phi). \tag{2}$$

2.1 Power Series Method

While solving the Schrödinger equation for different potentials, we will come across differential equations that can be put in the following form:

$$a(x)y'' + b(x)y' + c(x)y = 0, \tag{3}$$

where $a(x)$, $b(x)$, and $c(x)$ are polynomials and $y' = dy/dx$, $y'' = d^2y/dx^2$ are successive derivatives of an unknown function y . Such type of differential equations are generally solved using the power series method. We solve a simple differential equation $y' - 2y = 0$ to illustrate the power series method.

Assume that the unknown function y can be expanded in a power series as

$$y(x) = \sum_{n=0}^{\infty} a_n x^n. \tag{4}$$

Substituting for y in $y' - 2y = 0$, we obtain

$$\sum_{n=1}^{\infty} n a_n x^{n-1} - 2 \sum_{n=0}^{\infty} a_n x^n = 0, \tag{5}$$

which can be rewritten as

$$\sum_{n=0}^{\infty} (n+1) a_{n+1} x^n - \sum_{n=0}^{\infty} 2 a_n x^n = 0. \tag{6}$$

From the uniqueness of power series, we require the coefficient of each powers of x to vanish. For the coefficient of the x^n term,

We will encounter later in this article differential equations that can be put in the form of spherical Bessel equation, Legendre equation, and associated Laguerre equation. These differential equations are generally solved using the power series method.

we get, $(n + 1)a_{n+1} - 2a_n = 0$, which can be written as

$$a_{n+1} = \frac{2a_n}{n + 1}. \quad (7)$$

Using the above recursive relation, a_n can be expressed in terms of a_0 as follows:

$$a_n = \frac{2a_{n-1}}{n} = \frac{2^2 a_{n-2}}{n \cdot n - 1} = \dots = \frac{2^n a_0}{n!}. \quad (8)$$

Substituting (8) in (4) yields the solution for the unknown function y :

$$y(x) = \sum_{n=0}^{\infty} \frac{2^n a_0}{n!} x^n = a_0 \sum_{n=0}^{\infty} \frac{(2x)^n}{n!} = a_0 e^{2x}. \quad (9)$$

2.2 Particle on a Ring

Particle on a ring is a useful model for predicting the absorption properties of π -electrons of benzene.

Consider a particle of mass m_0 and energy E confined to the x - y plane under the influence of following potential:

$$V(r) = \begin{cases} 0 & r = R, \\ \infty & r \neq R. \end{cases} \quad (10)$$

This means that the r ($= R$) and θ ($= \pi/2$) coordinates of the particle are constants, while the ϕ coordinate is variable (see Figure 1). Thus the particle is only free to move on a ring of radius R in the x - y plane.

For $A = 0$ or $B = 0$, $e^{-im\phi}$ or $e^{im\phi}$ is a simultaneous eigenfunction of the Hamiltonian and the momentum, while for $A = B$ or $A = -B$, $\cos m\phi$ or $\sin m\phi$ is a simultaneous eigenfunction of the Hamiltonian and the parity.

Since the particle is confined to the ring, the wavefunction of the particle for $r \neq R$ is $\psi(\phi) = 0$.

On the ring, the potential is zero, and the Schrödinger equation (2) becomes

$$-\frac{\hbar^2}{2m_0 R^2} \frac{d^2 \psi(\phi)}{d\phi^2} = E \psi(\phi), \quad (11)$$

which can be rewritten as

$$\frac{d^2 \psi(\phi)}{d\phi^2} + m^2 \psi(\phi) = 0, \quad (12)$$

where $m = 2IE/\hbar^2$ with $I = m_0R^2$. The solution for the above equation can be given by

$$\psi(\phi) = Ae^{im\phi} + Be^{-im\phi}. \quad (13)$$

Now, a physically acceptable wave function must be single valued, i.e., $\psi(\phi) = \psi(\phi + 2\pi)$. Therefore,

$$Ae^{im\phi} + Be^{-im\phi} = Ae^{im\phi}e^{im2\pi} + Be^{-im\phi}e^{-im2\pi}, \quad (14)$$

which is true only if m is an integer: $m = 0, \pm 1, \pm 2, \dots$. Hence, the normalized eigenfunctions ($B=0$) and the corresponding energy eigenvalues are

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}, \text{ and } E_m = \frac{\hbar^2}{2I}m^2, \quad m = 0, \pm 1, \pm 2, \dots \quad (15)$$

We have shown eigenfunction corresponding to $m = 4$ and the energy level diagram in *Figure 2*. For a given value of integer m , eigenfunctions $(1/\sqrt{2\pi})e^{im\phi}$ and $(1/\sqrt{2\pi})e^{-im\phi}$ are degenerate and represent particle circling in opposite directions.

2.3 Particle on a Sphere

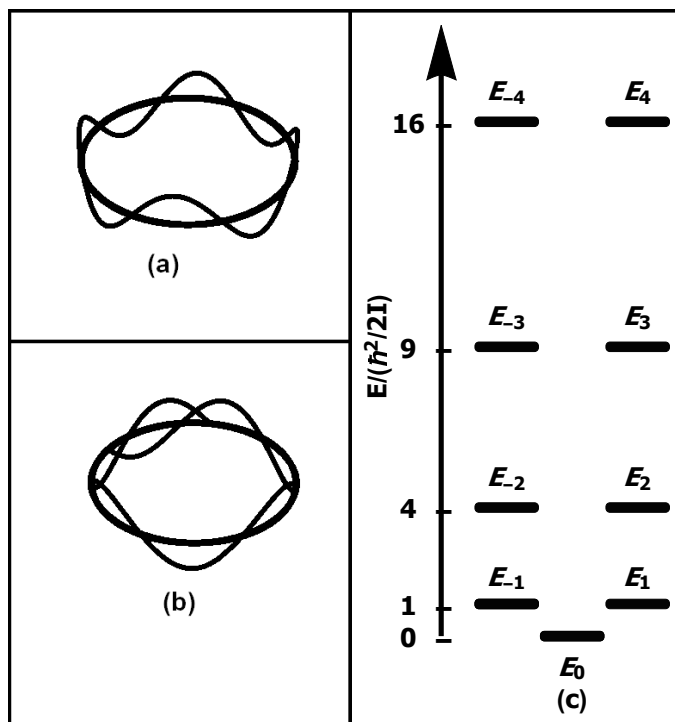
Consider a particle confined to the surface of a sphere of radius R . The potential is the same as in (10), but now the particle is allowed to move in three dimensions. For this case, the $r (=R)$ coordinate of the particle is constant, while θ and ϕ coordinates are variables. Thus, the Schrödinger equation (2) for a particle on a sphere takes the following form:

$$-\frac{\hbar^2}{2m_0R^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] Y(\theta, \phi) = EY(\theta, \phi). \quad (16)$$

Using the method of separation of variables, the above differential equation can be separated into two independent ordinary differential equations. First substituting $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$ in (16), and then multiplying both the sides by $\sin^2\theta$, and finally dividing both the sides by $Y(\theta, \phi)$ yields the following two differential equations:

Particle on a sphere model can explain the transition properties of π -electrons of fullerene C_{60} molecule. Here, we have to consider the splitting of degenerate energy levels under the icosahedral symmetry of the C_{60} molecule [4].

Figure 2. (a) Real part of the wavefunction $(1/\sqrt{2\pi})e^{im\phi}$ ($m = 4$) for a particle on a ring. (b) The wavefunction shown is unacceptable as it is not single valued. (c) Energy levels represented in units of $\hbar^2/2I$ for a particle on a ring. The ground state is non-degenerate, while all the other excited states are doubly-degenerate.



$$\frac{1}{\Phi(\phi)} \frac{d^2\Phi(\phi)}{d\phi^2} = -m^2; \quad (17)$$

$$\left[\sin(\theta) \frac{d}{d\theta} \left(\sin \theta \frac{d}{d\theta} \right) + \beta \sin^2 \theta - m^2 \right] \Theta(\theta) = 0, \quad (18)$$

where $\beta = 2IE/\hbar^2$ with $I = m_0R^2$, and m^2 is the separation constant.

(17) is same as particle on a ring case which has already been considered in the previous section. (18) can be solved using power series method and the solutions are known as associated Legendre function. Here parameter β has to be of the form:

$$\beta = l(l + 1), \quad l = 0, 1, 2, \dots \quad (19)$$

while

$$m = 0, \pm 1, \pm 2, \dots, \pm l \quad (2l + 1 \text{ values}). \quad (20)$$

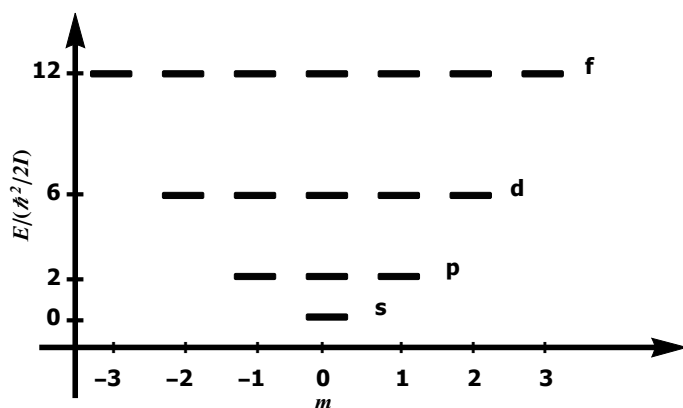


Figure 3. Energy levels represented in units of $\hbar^2/2I$ for a particle on a sphere. Symbols s, p, d, f represent states corresponding to the quantum numbers $l = 0, 1, 2,$ and 3 . The degeneracy of the energy level corresponding to the quantum number l is $2l + 1$.

We directly write the expression for $Y(\theta, \phi)$, also known as spherical harmonics [1]:

$$Y_l^m(\theta, \phi) = \epsilon \sqrt{\frac{(2l + 1)(l - |m|)!}{4\pi(l + |m|)!}} e^{im\phi} P_l^m(\cos \theta), \quad (21)$$

where $P_l^m(\cos \theta)$ is the associated Legendre function, $\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m \leq 0$. The energy eigenvalues are given by

$$E_l = \frac{\hbar^2 \beta}{2I} = \frac{\hbar^2}{2I} l(l + 1). \quad (22)$$

We have shown the energy level diagram for a particle on a sphere in *Figure 3*.

3. Spherically Symmetric Potentials

In this section, we will consider cases where all the three coordinates r, θ and ϕ are variables, and the potential depends only on the distance between the particle and the origin. Such potentials are called spherically symmetric potentials. The Schrödinger equation (2) for a spherically symmetric potential $V(r)$ can be written as:

$$-\frac{\hbar^2}{2m_0} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial^2}{\partial \phi^2} \right] \Psi(r, \theta, \phi) + V(r) \Psi(r, \theta, \phi) = E \Psi(r, \theta, \phi). \quad (23)$$

We can again use the method of separation of variables to separate the above differential equation into three independent ordinary differential equations. But it is convenient to club together the θ and ϕ part. To this end, we first substitute $\Psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$ in (23), and then multiply and divide both the sides by $-2m_0r^2/\hbar^2$ and $R(r)Y(\theta, \phi)$, respectively, which yields the following two differential equations:

$$\frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] = -l(l+1), \quad (24)$$

$$\frac{1}{R(r)} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) - \frac{2m_0r^2}{\hbar^2} (V(r) - E) = l(l+1), \quad (25)$$

where $l(l+1)$ is the separation constant. (24) is the angular part of the Schrödinger equation and has the same solution as particle on a sphere. (25) is the radial part of the Schrödinger equation, which can be rewritten as:

$$-\frac{\hbar^2}{2m_0r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2m_0r^2} \right] R(r) = ER(r). \quad (26)$$

The above equation is also known as the radial wave equation. Since the angular part is independent of the potential $V(r)$ and has already been discussed in Section 2.3, we need to only solve for the radial part for different potentials $V(r)$.

3.1 Particle in a Spherical Box

The interaction potential for a particle in a spherical box is given by:

$$V(r, \theta, \phi) = \begin{cases} 0 & \text{if } 0 < r < a, \\ \infty & r \geq a. \end{cases} \quad (27)$$

Since the particle cannot go outside the spherical box, we have

$$\Psi(r, \theta, \phi) = 0 \quad \text{for } r \geq a. \quad (28)$$

Inside the box, the radial wave equation (26) reads

$$-\frac{\hbar^2}{2m_0 r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) + \frac{\hbar^2 l(l+1)}{2m_0 r^2} R(r) = ER(r). \quad (29)$$

We substitute

$$r = \frac{\rho}{k}, \quad \text{where } k = \frac{\sqrt{2m_0 E}}{\hbar}, \quad (30)$$

in (29), and perform some algebraic manipulations to bring it in the following form:

$$\rho^2 \frac{d^2 R(\rho)}{d\rho^2} + 2\rho \frac{dR(\rho)}{d\rho} + [\rho^2 - l(l+1)] R(\rho) = 0. \quad (31)$$

This equation is known as spherical Bessel equation, and the solutions are called spherical Bessel function. The boundary condition $R(a) = 0$ yields $ka = \beta_{l,n}$, where $\beta_{l,n}$ denotes the n^{th} root of l^{th} order Bessel function. The total wave function, the product of the radial and the angular wave function, is thus given by [5]:

$$\Psi_{n,l,m}(r, \theta, \phi) = A j_l \left(\frac{\beta_{l,n}}{a} r \right) Y_{l,m}(\theta, \phi), \quad (32)$$

where A is the normalization constant, and j_l is the spherical Bessel function of the first kind. Also, energy eigenvalues can be expressed as:

$$E_{l,n} = \frac{\hbar^2 k^2}{2m_0} = \frac{\hbar^2 \beta_{l,n}^2}{2m_0 a^2}. \quad (33)$$

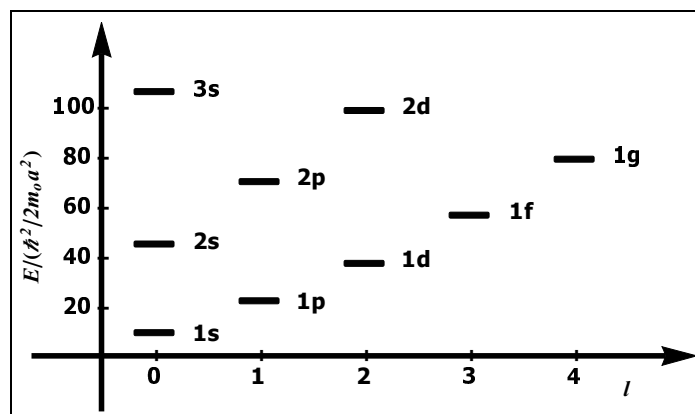
Figure 4 shows a few of the lowest energy eigenvalues, and Table 1 lists the numerical values of the energy levels.

3.2 Isotropic Three-dimensional Harmonic Oscillator

The interaction potential for the three-dimensional isotropic harmonic oscillator is given by:

$$V(r) = \frac{1}{2} m_0 \omega^2 r^2. \quad (34)$$

Figure 4. Lowest energy levels for particle in a spherical box of radius a . Since energy is represented in units of $\hbar^2/2m_0a^2$, the numerical values represent the magnitude of $\beta_{l,n}^2$ (see Table 1).



$n \backslash l$	0	1	2	3	4
1	9.87	20.19	33.22	48.83	66.95
2	39.48	59.68	82.72	108.52	137.00
3	88.83	118.90	151.86	187.64	226.19
4	157.91	197.86	240.70	286.41	334.94

Table 1. Numerical values of $\beta_{l,n}^2$ for different (l, n) pairs.

The solution for the radial wave equation (26) can be written as [6]:

$$\Psi_{k,l}(r) = Ar^l e^{-\beta^2 r^2/2} L_k^{l+1/2}(\beta^2 r^2), \quad (35)$$

where A is the normalization constant, $L_k^{l+1/2}(\beta^2 r^2)$ is associated Laguerre polynomial, and $\beta = \sqrt{m_0 \omega / \hbar}$. The total wave function is simply the product of the radial wave function (35) and the angular wave function (21).

The energy eigenvalues can be expressed as

$$E_{k,l} = \hbar \omega \left(2k + l + \frac{3}{2} \right), \quad (36)$$

where k and l are non-negative integers. Substituting $2k + l = n$,

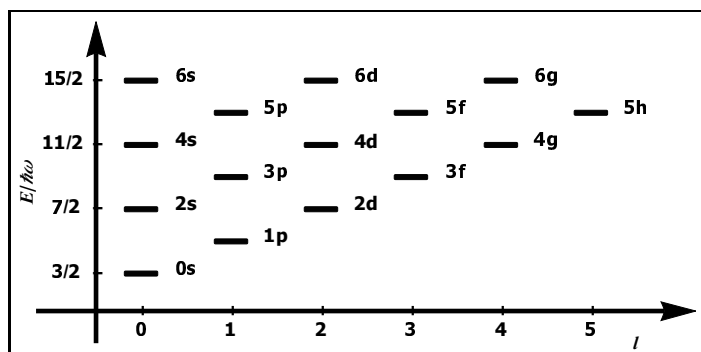


Figure 5. Energy level diagram for isotropic three-dimensional harmonic oscillator. For even n , possible values of l are $0, 2, \dots, n - 2, n$; and for odd n , possible values of l are $1, 3, \dots, n - 2, n$. For both the even and odd cases, the degeneracy of the n^{th} energy level is $\frac{(n + 1)(n + 2)}{2}$.

(36) becomes

$$E_n = \hbar\omega \left(n + \frac{3}{2} \right). \quad (37)$$

For even n , quantum number l can take the following values:

$$l = 0, 2, \dots, n - 2, n, \quad (38)$$

while for odd n ,

$$l = 1, 3, \dots, n - 2, n. \quad (39)$$

Figure 5 shows a few of the lowest energy eigenvalues. To calculate the degeneracy of the n^{th} energy level, we take into account the $2l+1$ degeneracy of the l quantum number. A simple summation leads to the following results for the even and odd cases:

$$\sum_{l=0,2,\dots,n-2,n} (2l + 1) = \frac{(n + 1)(n + 2)}{2}, \quad \text{if } n \text{ is even,} \quad (40)$$

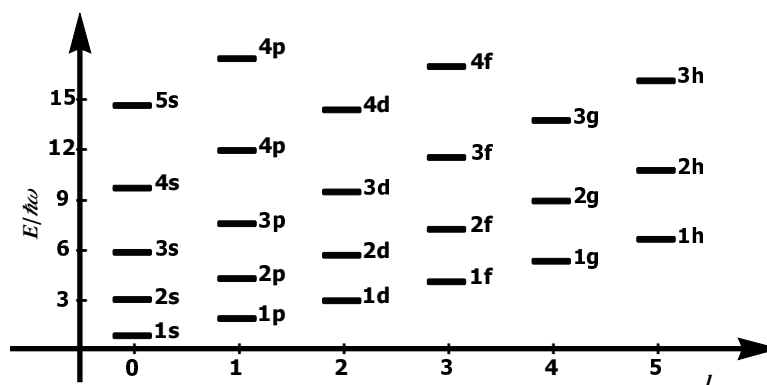
$$\sum_{l=1,3,\dots,n-2,n} (2l + 1) = \frac{(n + 1)(n + 2)}{2}, \quad \text{if } n \text{ is odd.} \quad (41)$$

3.3 Spherically Confined Isotropic Three-dimensional Harmonic Oscillator

The interaction potential for the spherically confined isotropic three-dimensional harmonic oscillator is given by:

$$V(r) = \begin{cases} \frac{1}{2}m_0\omega^2r^2 & r < a, \\ \infty & r \geq a. \end{cases} \quad (42)$$

Figure 6. Energy level diagram for spherically confined isotropic three-dimensional harmonic oscillator. Here the confinement radius is taken to be 3 units (in units of $\sqrt{\hbar/m_0\omega}$).



For $r \geq a$, the wavefunction $\Psi(r, \theta, \psi) = 0$.

For $r < a$, the solution to the radial wave equation (26) can be written as [7]:

$$R_{n,l}(r) = Nr^l e^{-\beta^2 r^2/2} {}_1F_1\left(\frac{2l+3}{4} - \frac{E_{n,l}}{2\hbar\omega}, l + \frac{3}{2}, \beta^2 r^2\right), \quad (43)$$

where ${}_1F_1$ is the confluent hypergeometric function, and $\beta = \sqrt{m_0\omega/\hbar}$. The total wave function is given as the product of the radial wave function (43) and the angular wave function (21). The boundary condition requires the radial wave function to vanish at $r = a$:

$${}_1F_1\left(\frac{2l+3}{4} - \frac{E_{n,l}}{2\hbar\omega}, l + \frac{3}{2}, \beta^2 a^2\right) = 0. \quad (44)$$

For a fixed l , values of energy, where ${}_1F_1$ vanishes, correspond to the energy eigenvalues of the confined harmonic oscillator. *Figure 6* shows a few of the energy levels and *Table 2* lists their magnitude. We can see from the figure that as we consider higher energy levels for a given l , the difference between successive energy levels increases.

4. Heat Capacity of Endohedral Fullerenes

We take He@C₆₀ as our endohedral fullerene where helium atom is enclosed inside C₆₀ (see *Figure 7*). Two different quantum models have been considered to compute the heat capacity of He@C₆₀. We have assumed the following for each of the quantum models:

Table 2. Energy eigenvalues in units of $\hbar\omega$ for different (l, n) pairs.

$n \backslash l$	0	1	2	3	4	5
1	1.50	2.53	3.60	4.73	5.94	7.25
2	3.66	4.91	6.31	7.85	9.53	11.35
3	6.47	8.18	10.07	12.13	14.33	16.69
4	10.30	12.56	14.96	17.55	20.29	23.19
5	15.23	18.01	20.97	24.09	27.38	30.82

1. Spherical well model

- Helium atom cannot get outside the fullerene cage.
- It does not feel any force inside the cage.

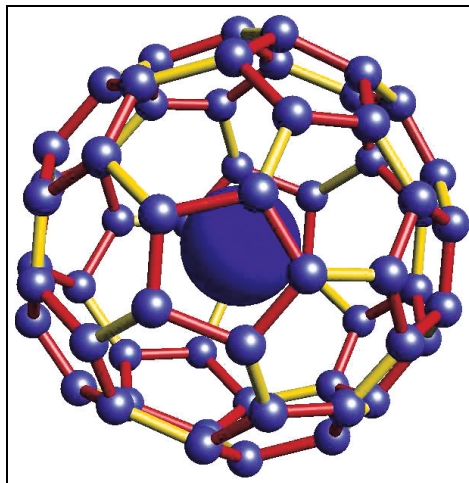
2. Spherically confined three-dimensional harmonic oscillator model

- Helium atom cannot get outside the fullerene cage.
- It feels linear force akin to harmonic oscillator inside the cage.

Moreover, both the models consider helium atom as a point particle. Expressions for the energy levels are provided in (33) and (44) for spherical well and confined three-dimensional harmonic oscillator potentials. We can obtain the numerical values of the energy levels after providing the values of different parameters corresponding to He@C₆₀. We use the following expression for computing the specific heat capacity, written in terms of first and second moments of energy:

$$C_v = \frac{\partial \langle E \rangle}{\partial T} = \frac{1}{k_B T^2} (\langle E^2 \rangle - \langle E \rangle^2). \quad (45)$$

Figure 7. Endohedral fullerene: A helium atom inside C_{60} molecule.



It is important to take into account the degeneracy of energy levels while calculating the heat capacity. The numerical results [8, 9] of the heat capacity for both of these models are shown in *Figure 8*.

Of these two models, results for the confined harmonic oscillator corroborate with the computational results obtained from Hartree–Fock and density functional theory (DFT) methods available in Gaussian software [9].

5. Conclusions

Thus, simplified models, which retain important features, help predict results, as shown by the confined harmonic oscillator quantum model of the endohedral fullerene. A natural progression along similar lines is to set up simple quantum models for systems like carbon nanotube, which has cylindrical symmetry.

Further, one can relate the degeneracies of the energy eigenvalues to the symmetry of the system. To this end, group theory is a powerful tool to study the relation between symmetries of the system and the degeneracies of the energy levels. For example, $SO(3)$ symmetry corresponding to the interaction potential of a particle on a sphere leads to $2l + 1$ degeneracy of l^{th} energy level. Sim-



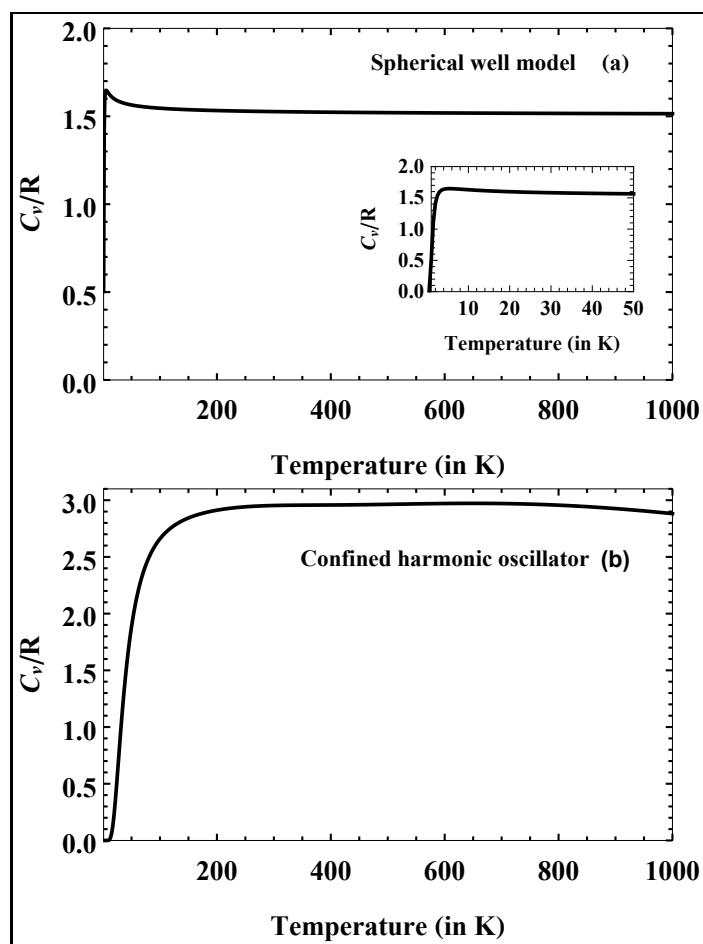


Figure 8. (a) The heat capacity increases rapidly and goes above 1.5 R attaining a maximum around 6 K, as can be seen in the inset. It then levels off to a value of 1.5 R in the high-temperature limit. This result is reminiscent of the fact that each degree of freedom contributes $R/2$ in the high-temperature limit.

(b) The heat capacity starts rising from zero and reaches 3 R in the considered temperature range. This is due to the fact that the spacing between lower energy levels of a confined harmonic oscillator is similar to that of a harmonic oscillator.

ilarly, $SU(3)$ symmetry of isotropic three-dimensional harmonic oscillator results in $(n+1)(n+2)/2$ degeneracy of n^{th} energy level.

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Suggested Reading

Address for Correspondence
Chandan Kumar
Department of Physical
Sciences,
Indian Institute of Science
Education and Research
(IISER) Mohali,
Knowledge City SAS Nagar,
Sector 81,
Mohali 140 306, Punjab.
Email:
chandankumar@iisermohali.
ac.in

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